=> screen 963

L1 SCREEN CREATED

=> screen 1821 OR 1822 OR 1823 OR 1824

L2 SCREEN CREATED

=>
Uploading C:\Program Files\Stnexp\Queries\09676487-b.str

L3 STRUCTURE UPLOADED

=> que L3 AND L1 AND L2

L4 QUE L3 AND L1 AND L2

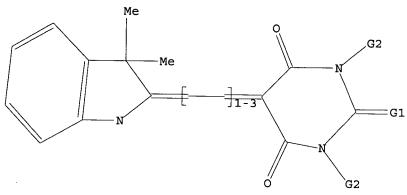
=> d

L4 HAS NO ANSWERS

L1 SCR 963

L2 SCR 1821 OR 1822 OR 1823 OR 1824

L3 STR



G1 0,S

G2 H, Cb, Hy, Ak, Ph

G3 H, Ak

Structure attributes must be viewed using STN Express query preparation. L4 QUE ABB=ON PLU=ON L3 AND L1 AND L2

=> s 14 sss sam

SAMPLE SEARCH INITIATED 11:18:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED

5 ITERATIONS

4 ANSWERS

Munch Search

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

5 TO 234

PROJECTED ANSWERS:

4 TO 200

4 SEA SSS SAM L3 AND L1 AND L2

L5

=> d

L5 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2003 ACS

RN 521060-32-2 REGISTRY

CN 4,6(1H,5H)-Pyrimidinedione, 5-[(2E,4Z)-4-(1,3-dihydro-1,3,3-trimethyl-2H-indol-2-ylidene)-2-butenylidene]dihydro-1,3-dimethyl-2-thioxo-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H23 N3 O2 S

SR CA

LC STN Files: CA, CAPLUS

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1957 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

=> FIL CAPLUS HCAPLUS USPATFULL USPAT2 COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

3.28 3.49

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FILE 'USPAT2' ENTERED AT 11:20:37 ON 26 JUN 2003 CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

=> d his

(FILE 'HOME' ENTERED AT 11:18:10 ON 26 JUN 2003)

FILE 'REGISTRY' ENTERED AT 11:18:22 ON 26 JUN 2003 L1 SCREEN 963 L2SCREEN 1821 OR 1822 OR 1823 OR 1824 L3 STRUCTURE UPLOADED L4QUE L3 AND L1 AND L2 L5 4 S L4 SSS SAM FILE 'CAPLUS, HCAPLUS, USPATFULL, USPAT2' ENTERED AT 11:20:37 ON 26 JUN => s 15L6 8 L5 => duplicates remove 16 DUPLICATE PREFERENCE IS 'CAPLUS, HCAPLUS' KEEP DUPLICATES FROM MORE THAN ONE FILE? Y/(N):n PROCESSING COMPLETED FOR L6 L74 DUPLICATE REMOVE L6 (4 DUPLICATES REMOVED) => d 17 1-4 ibib abs hitstr ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS L7 DUPLICATE 1 ACCESSION NUMBER: 2003:193710 CAPLUS DOCUMENT NUMBER: 138:350727 TITLE: Solvent-sensitive dyes to report protein conformational changes in living cells AUTHOR (S): Toutchkine, Alexei; Kraynov, Vadim; Hahn, Klaus CORPORATE SOURCE: Department of Cell Biology, Scripps Research Institute, La Jolla, CA, 92037, USA SOURCE: Journal of the American Chemical Society (2003), 125(14), 4132-4145 CODEN: JACSAT; ISSN: 0002-7863 PUBLISHER: American Chemical Society DOCUMENT TYPE: Journal LANGUAGE: English Covalent attachment of solvent-sensitive fluorescent dyes to proteins is a powerful tool for studying protein conformational changes, ligand binding, or posttranslational modifications. We report here new merocyanine dyes that make possible the quantitation of such protein activities in individual living cells. The quantum yield of the new dyes is sharply dependent on solvent polarity or viscosity, enabling them to report changes in their protein environment. This is combined with other stringent requirements needed in a live cell imaging dye, including appropriate photophys. properties (excitation >590 nm, high fluorescence quantum yield, high extinction coeff.), good photostability, minimal aggregation in water, and excellent water soly. The dyes were derivatized with iodoacetamide and succinimidyl ester side chains for site-selective covalent attachment to proteins. A novel biosensor of Cdc42 activation made with one of the new dyes showed a 3-fold increase in fluorescence intensity in response to GTP-binding by Cdc42. The dyes reported here should be useful in the prepn. of live cell biosensors for a diverse range of protein activities. TТ 521060-32-2P RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation) (solvent-sensitive dyes to report protein conformational changes in living cells) RN 521060-32-2 CAPLUS 4,6(1H,5H)-Pyrimidinedione, 5-[(2E,4Z)-4-(1,3-dihydro-1,3,3-trimethyl-2H-CN

indol-2-ylidene)-2-butenylidene]dihydro-1,3-dimethyl-2-thioxo- (9CI) (CA

Double bond geometry as shown.

INDEX NAME)

$$R_{1,2} = mc$$

$$Q_3 = S$$

$$m = Z$$

$$R^h = Me$$

$$R^{d-g} = H$$

REFERENCE COUNT:

THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS

72

DUPLICATE 2

ACCESSION NUMBER: DOCUMENT NUMBER:

1996:693723 CAPLUS

TITLE:

125:312364

Silver halide photographic materials containing

hexamethinemerocyanine compounds Sakurada, Masami; Oono, Shigeru Fuji Photo Film Co Ltd, Japan

PATENT ASSIGNEE(S):

Jpn. Kokai Tokkyo Koho, 33 pp.

SOURCE:

CODEN: JKXXAF Patent

DOCUMENT TYPE: LANGUAGE:

GΙ

INVENTOR(S):

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE -----JP 08211552 A2 19960820 JP 1995-15010 19950201 PRIORITY APPLN. INFO.: JP 1995-15010 19950201

$$R^{2}$$
 R^{3} $L^{1}L^{2} = L^{3}L^{4} = L^{5}L^{6}$ R^{2} R^{3} R^{3}

The title materials comprise a hydrophilic colloid layer contg. . $\operatorname{\mathsf{gtoreq.1}}$ AB hexamethinemerocyanine compd. I [Z1 = nonmetal atoms required to form a benzo-condensed or naphtho-condensed ring; M = H, atoms or metal atom forming a monovalent cation; n = 1-3; R1-3 = (substituted) alkyl; L1-6(substituted) methine group, the adjacent substituents may condensed to form a 5- or 6-membered ring; Z2 = atoms required to form a (substituted) heterocycle selected from pyrazolidinedion, isooxazolone, pyrazolopyridone, barbituric acid, pyridone, rhodanine]. The compds. are stable and water-sol. and provide photog. materials showing improved decoloring properties without adverse effects on the photog. properties. IT183272-29-9

RL: DEV (Device component use); USES (Uses)

(Ag halide photog. materials contg. hexamethinemerocyanine compds.)

183272-29-9 CAPLUS RN

1,4-Benzenedisulfonic acid, 2-[5-[6-[1,3-dihydro-1,1-dimethyl-7-sulfo-3-(4-CNsulfobuty1)-2H-benz[e]indol-2-ylidene]-2,4-hexadienylidene]tetrahydro-2,4,6-trioxo-3-(2-sulfoethyl)-1(2H)-pyrimidinyl]-, pentapotassium salt (9CI) (CA INDEX NAME)

5 K

1.7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS DUPLICATE 3

ACCESSION NUMBER:

1996:640204 CAPLUS

DOCUMENT NUMBER:

125:278576

TITLE:

Molecular hyperpolarizabilities of barbituric acid and

cyclobutene-1,2-dione derivatives. Electronic and

steric effects

AUTHOR (S):

Cho, Bong Rae; Je, Jong Tae; Lee, Seung Jae; Lee, Sang

Hae; Kim, Hyun Soo; Jeon, Seung Joon; Song, Ok-Keum;

Wang, C. H.

CORPORATE SOURCE:

Department of Chemistry, Korea University, Seoul,

136-701, S. Korea

SOURCE:

Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1996), (10), 2141-2144

CODEN: JCPKBH; ISSN: 0300-9580

PUBLISHER:

Royal Society of Chemistry

DOCUMENT TYPE:

Journal LANGUAGE: English

A series of merocyanine dyes contg. various donors and barbituric acid and AB cyclobutene-1,2-dione moieties as the acceptors have been synthesized and their first-order hyperpolarizabilities .beta. were detd. The .beta. values of the barbituric acid derivs. increase as the strength of the donor is increased from 4-(dimethylamino)phenyl to trimethylindolinyl to benzothiazolinyl, apparently due to the gradual decrease in the bond length alteration from a large pos. value to an optimum one by a stronger donor. In contrast, the .beta. values for the cyclobutene-1,2-dione derivs. decrease with the same variation of the donors even though the cyclobutene-1,2-dione is a poorer acceptor than the barbituric acid moiety. The results have been attributed to the electron-donating ability of the donors and the increased distortion of the chromophores from planarity.

IT 93818-94-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (hyperpolarizabilities of merocyanines from barbituric acid and cyclobutenediones)

RN 93818-94-1 CAPLUS

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[(1,3-dihydro-1,3,3-trimethyl-2H-indol-CN2-ylidene)ethylidene]- (9CI) (CA INDEX NAME)

03= " T

ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

1963:426202 CAPLUS

DOCUMENT NUMBER:

59:26202

ORIGINAL REFERENCE NO.:

59:4716e-q

TITLE:

Stereochemical factors affecting optical sensitization

AUTHOR(S): CORPORATE SOURCE:

Anderson, G. de W.

Imp. Chem. Inds. Ltd., Manchester, UK

SOURCE:

Sci. Phot., Proc. Intern. Colloq., Liege (1962), 1959,

487-511

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

GI For diagram(s), see printed CA Issue.

The formation of polymeric forms (J aggregates contg. at least 150 mols.) AB of sensitizing dyes in Ag halide emulsions is studied. The positions of the absorption max. in MeOH and in the emulsion are given for a large no. of merocyanines. Symmetry of the terminal groups and, in general, redn. of the no. of possible stereoisomers, promotes the J aggregation. Electronic rather than structural symmetry is an essential, but not the sole requirement. Malononitrile dimethinemerocyanines with 2 stereo forms show J-band aggregation. N,N'-Diethylthioharbituric acid dimethinemerocyanines show aggregation only when a single isomer is possible. The no. of stereoisomers can be limited by enclosing the polymethine chain in a cyclic system. Even highly similar d and I forms increase this no. and prevent J-band sensitization. A new 4,7'-quinocyanine of structure I is described.

93818-94-1, Barbituric acid, 5-[2-(1,3,3-trimethyl-2-IT indolinylidene)ethylidene]-

(photographic sensitization by, stereoisomerism and)

93818-94-1 CAPLUS RN

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[(1,3-dihydro-1,3,3-trimethyl-2H-indol-CN2-ylidene)ethylidene]- (9CI) (CA INDEX NAME)